Variations of Pairing Potential and Charge Distribution in Presence of a Non-magnetic Impurity

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Abstract

Using an attractive Hubbard model we examine spatial variations of superconducting order parameter and local charge on a two dimensional lattice. For various band filling we show the effect of destruction of the order parameter around a non-magnetic impurity. In case of a half-filled system such destruction is accompanied by appearance of characteristic charge variations around the impurity with an isotropic distribution.

Key words: superconductivity, non-magnetic impurities, charge density wave

According to Anderson theorem the effect of non-magnetic disorder on s-wave superconductors can be neglected unless spatial fluctuations of order parameter are present [1,2]. However this theorem invented for conventional superconductors cannot be applied to other superconductors with a short coherence length [3,4] and for those of anisotropic pairing [5]. Another interesting situation, where the influence of disorder can be important, has been found in a case with an interplay between different long range orders like superconductivity and charge density wave (CDW). In a negative U Hubbard model this happens for half-filling [6]. Here finite disorder favours superconducting phase against CDW [3,7,8,9]. These results show that the effect of disorder on superconductivity can be sometimes beneficial leading to disorder induced superconductivity [9]. It must be also noticed that the charge ordering mechanism and its interplay with superconductivity are of a great interest itself because of existence of charge strips in HTc superconductors [10]. In the present note we will examine the effect of a single impurity on a superconducting order parameter and charge fluctuations around non-magnetic impurity in a two dimensional lattice.

We start from negative U Hubbard hamiltonian [3,4,11]:

$$H = -t \sum_{\langle i,j \rangle \sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + h.c. \right) + \sum_{i\sigma} \left(\epsilon_i - \mu \right) c^{\dagger}_{i\sigma} c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where ϵ_i denotes an impurity potential located at the central site $i=0$ ($\epsilon_i = \epsilon_0 \delta_{0,i}$) and U on–site attraction ($U<0$) which is the same at each lattice site i.

Our actual calculations consist of solving, self-consistently, the following Bogoliubov-de Gennes equation [12]:

$$\sum_j \begin{pmatrix} (E^{\nu} - \varepsilon_i + \mu)\delta_{ij} + t_{ij} & \Delta_i \delta_{ij} \\ \Delta^{*}_i \delta_{ij} & (E^{\nu} + \varepsilon_i - \mu)\delta_{ij} - t_{ij} \end{pmatrix} \begin{pmatrix} u^{\nu}_j \\ v^{\nu}_j \end{pmatrix} = 0\,, \tag{2}$$

where $\varepsilon_i = \epsilon_i + U n_i/2$ denotes the renormalized site energy. The pairing potential Δ_i and the local charge n_i are to be found self-consistently:

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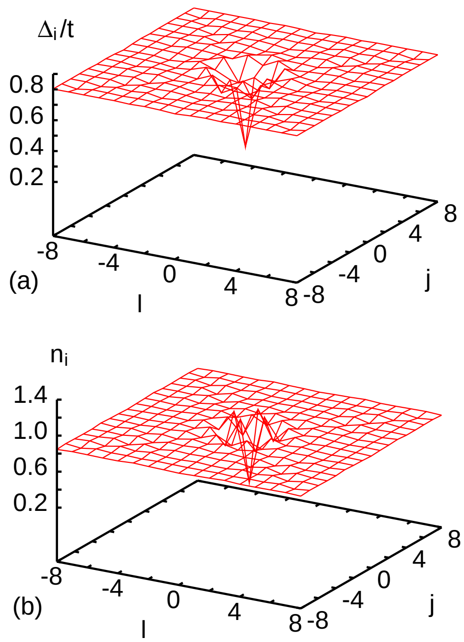

Fig. 1. Pairing potential Δ_i (a) and charge n_i ($i =< l, j >$) on a two dimensional lattice around the central impurity ($U = -3t$, $n = 0.85$, $\epsilon_0 = t$ at $(l, j) = (0, 0)$).

$$\Delta_i = -U \sum_{\nu} u_i^{\nu} v_i^{\nu *} (1 - 2f(E^{\nu})) ,$$
$$n_i = 2 \sum_{\nu} (|u_i^{\nu}|^2 f(E^{\nu}) + |v_i^{\nu}|^2 (1 - f(E^{\nu}))) , \tag{3}$$

where ν enumerates the solutions of Eq. 2 for a given band filling n.

To examine the effect of a single impurity on the surrounding lattice sites we have solved the above equations (2,3) in the real space using the recursion Lanczos algorithms for a superconductor [13]. In Fig. 1 we show the local distributions of the pairing potential Δ_i (Fig. 1a) and the charge n_i (Fig. 1b) around impurity located in the center of a 2d lattice for a band filling n close but slightly smaller than a half-filed situation ($n = 0.85$). Due to the impurity ($\epsilon_0 = t$) the pairing potential Δ_i is going down rapidly at the central site (Fig. 1a). This change is coupled to variation of the local charge n_i (Fig. 1b). Note that both distributions of Δ_i and n_i have similar form e.g. they show similar anisotropy. The situation is quite different for a half filled system $n = 1$ (Fig. 2). Note that in this case the paring potential goes down around impurity more smoothly and isotropically (Fig. 2a) in comparison to the previous case (Fig. 1a). Interestingly, destruction of pairing is associated with strong oscillation of charge n_i (Fig. 2b). It is clear that around the central impurity the electron charge form a localized wave, with a characteristic size of 8-9 lattice spaces. In case

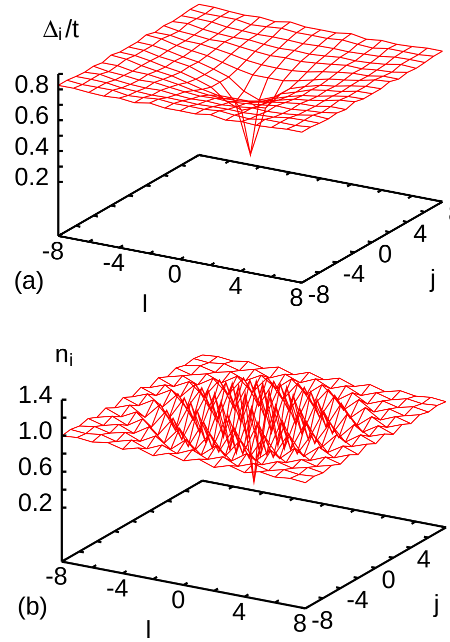

Fig. 2. Pairing potential Δ_i (a) and charge n_i ($i =< l, j >$) on a two dimensional lattice around the central impurity ($U = -3t$, $n = 1.0$, $\epsilon_0 = t$ at $(l, j) = (0, 0)$).

of finite concentration of impurities we can expect superconductor with islands of a normal phase [11]. Our calculations show the appearance of local CDW. That in turn indicates that impurities can contribute to a phase separation phenomenon [9].

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